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LETTER TO THE EDITOR

A numerical test of the conjectured exact S-matrix of the 2D Ising model in a magnetic field

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Abstract. The finite-size scaling functions of the correlation lengths in the 2D Ising model in a magnetic field are calculated numerically. The asymptotic behaviour in the limit of large scaling variables is studied and can be used to estimate the particle masses and coupling constants of the underlying effective field theory. The results are consistent with the conjectured minimal S-matrix obtained from the conformal bootstrap.

In two dimensions, the principle of conformal invariance allows a detailed description of critical statistical systems. Results include the exact determination of the central charge, critical exponents and correlation functions for numerous physical systems [1].

It is natural to ask whether conformal invariance at the critical point could be used to describe the system in the entire scaling region which is no longer scale-invariant but where the correlation lengths are still much larger than the interatomic distances. Indeed, it was shown by Zamolodchikov [2] that if the critical point Hamiltonian is perturbed by one of the relevant scaling fields φ_{12}, φ_{21} or φ_{13} (where the indices are the usual Kac labels) the off-critical system may possess integrals of motion Q_s of spin s, built from $T(z)$ and its derivatives, where $T(z)$ is the energy–momentum tensor. This implies that the S-matrix factorizes in terms of two-particle scattering amplitudes which must satisfy the Yang–Baxter equations, bootstrap requirements, unitarity and crossing symmetry. Solving these requirements then allows us to conjecture [2] an S-matrix which should describe the off-critical theory under consideration. In the example of the 2D Ising model in a magnetic field (to which we restrict ourselves in the sequel), the effective theory whose S-matrix one is going to construct turns out to contain eight stable massive particles with the mass spectrum [2]

$$\begin{aligned}
m_2/m_1 &= 2\cos\pi/5 = 1.618\,0339\ldots\\
m_3/m_1 &= 2\cos\pi/30 = 1.989\,0437\ldots\\
m_4/m_1 &= 2m_2\cos 7\pi/30 = 2.404\,8671\ldots\\
m_5/m_1 &= 2m_2\cos 2\pi/15 = 2.956\,2952\ldots\\
m_6/m_1 &= 2m_2\cos\pi/30 = 3.218\,3404\ldots\\
m_7/m_1 &= 4m_2\cos\pi/5\cos 7\pi/30 = 3.891\,1568\ldots\\
m_8/m_1 &= 4m_2\cos\pi/5\cos 2\pi/15 = 4.783\,3861\ldots.
\end{aligned}\qquad (1)$$

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This result is believed to indicate a relation to E_8, since the values of s for which integrals of motion are known to exist coincide with the exponents of E_8 modulo 30, its Coexter number. Also the coset construction $(E_8)_1 \otimes (E_8)_1/(E_8)_2$ gives a central charge $c = \frac{1}{2}$. The possibility of a relationship with the E_8 affine Toda theory has been discussed at length (see e.g. [3–5]) although it is now believed that, for example, the S-matrices of the 2D Ising model in a magnetic field and of the affine E_8 Toda theory with *real* couplings are different [6].

The predictions for the masses m_1, m_2, m_3 were confirmed numerically [7–9] which adds confidence that the assumptions leading to (1) should be satisfied in physical systems. However, no direct numerical checks on the S-matrix, testing for example coupling constants, have yet been performed which do not from the outset assume integrability (see also below).

Similar mass predictions exist for many other conformal systems perturbed with φ_{12}, φ_{21} or φ_{13} (for mass ratios and 'minimal' S-matrices see e.g. [5, 10] and references therein) and were confirmed numerically in systems as different as the tricritical Ising model [11, 12, 13], the three-states Potts model [14, 15], the Ashkin–Teller model [13] or the Yang–Lee edge singularity [15, 16]. Further, numerical calculations on the mass spectrum of the tricritical Ising model [17] and the Ashkin–Teller model [18] perturbed with the order parameter (φ_{22}) appear to reproduce the mass spectrum (1) below the continuum threshold, although no integrals of motion Q_s with $s \neq 1$ are known. This latter observation is yet to be understood. In spite of these numerical confirmations, the S-matrices obtained are by no means uniquely determined. It is well known that the requirements mentioned above only fix the S-matrix up to so-called CDD-factors [19]. The presence of these factors in the S-matrix does not modify the mass spectrum but may change the coupling constants [5, 6, 10, 19]. It is therefore of interest to be able to distinguish at least numerically between different S-matrices with the same mass spectrum.

In this letter, we report numerical calculations of the 2D Ising model in a magnetic field which improve on previous tests [7–9] on the mass spectrum. Further, we shall compare the asymptotic behaviour of the finite-size scaling functions with the predictions from S-matrix theory. Our results are fully consistent with the minimal S-matrix proposed by Zamolodchikov [2], that is, we do not see evidence for the presence of CDD-factors in this particular model. Our findings are also in agreement with analytical studies using the thermodynamic Bethe ansatz [15, 20], but in contradistinction to these methods, we do not have to make any assumptions on the integrability of the system.

The following method of analysis will be used. Lüscher [21] has shown how to relate mass shifts of a field theory in a finite volume to the scattering amplitude, studying theories with simple mass spectra, in particular theories where the one-particle states all have the same mass. This was confirmed numerically for the 4D Ising model [22] and for the 2D $O(3)$ nonlinear sigma model [23]. Klassen and Melzer [24] have generalized the results of [21] to the case of n massive particles which may have different masses. We merely quote their fairly general results to the extent needed here and refer to their paper [24] for further details and a precise statement of the technical assumptions to be made.

For simplicity, we only consider two-dimensional systems in a slab of finite length L. Let $a = 1, \ldots, n$ denote the n stable particles and let $0 < m_1 < m_2 < \ldots < m_n$ be their masses. Then the mass shift $\Delta m_a(L) = m_a(L) - m_a$ is for states with mass $m_a < 2m_1$ [24]

$$\Delta m_a(L)/m_1 = M_a^{(1)} + M_a^{(2)} + \mathrm{O}(\exp(-\sigma_a L)) \tag{2}$$

$$M_a^{(1)} = -\frac{1}{8m_a^2} \sum_{\substack{b,c \\ |m_b^2 - m_c^2| < m_a^2}} \frac{\lambda_{abc}^2}{\mu_{abc}} \exp(-\mu_{abc} L) \tag{3}$$

$$M_a^{(2)} = -\frac{1}{2\pi} \sum_b{}' \int_{-\infty}^{\infty} \mathrm{d}\theta \exp(-\cosh\theta\, m_b L) m_b \cosh\theta \left(S_{ab}\left(\theta + \frac{\mathrm{i}\pi}{2}\right) - 1 \right) \tag{4}$$

where $\mu_{abc} = m_b m_c m_a^{-1} \sin u_{bc}^a$, u_{bc}^a is defined by $m_a^2 = m_b^2 + m_c^2 + 2m_b m_c \cos u_{bc}^a$ and

$$\lambda_{abc}^2 = -8\mathrm{i}(m_b m_c \sin u_{bc}^a)^2 \,\mathrm{Res}_{\theta = \mathrm{i}u_{bc}^a} S_{bc}(\theta) \tag{5}$$

where $S_{ab}(\theta)$ is the two-particle S-matrix describing the scattering process $ab \to ab$ and θ is the rapidity variable. The prime in (4) indicates that one should only sum over terms which are larger than the error term $\mathrm{O}(\exp(-\sigma_a L))$. The exact size of the error coefficient will be discussed in [24]. σ_a is never bigger (and occasionally a bit smaller) than $2\mu_{a11}$. Note that these relations were derived without assuming any particular form of the Lagrangian of the theory considered. Knowing the S-matrix, one can derive numerical values for μ_{abc} and λ_{abc}. In table 1, we list the contributions to $M_a^{(1)}$ which correspond to *simple* poles of the minimal S-matrix (that is, without CDD-factors) first conjectured by Zamolodchikov [2, 5, 24]. The values of table 1 with $\mu_{abc} < 2\mu_{a11}$ are those we are going to use to calculate $M_a^{(1)}$ and which will be compared to our numerical results below.

A convenient technique to accurately calculate the scaling functions of the masses $\tilde{m}_i$ or inverse correlations length ξ_i^{-1} consists of diagonalizing the transfer matrix on finite lattices. Computationally, it is advantageous to consider the extreme anisotropic limit where the transfer matrix reduces to the exponential of the quantum Hamiltonian (for a review and a discussion of the numerical techniques see [25])

$$H = -\sum_{n=1}^{N} (t\sigma^z(n) + \sigma^x(n)\sigma^x(n+1) + h\sigma^x(n)) \tag{6}$$

where the σ are the Pauli matrices and periodic boundary conditions are used. N is the number of sites, t is related to the temperature and h is related to the magnetic

Table 1. Numerical values for μ_{abc} and $\rho_{abc} = \lambda_{abc}^2/(8m_a^2\mu_{abc})$ as obtained from the simple poles of the minimal E_8 S-matrix corresponding to the 2D Ising model in a magnetic field.

	abc	μ_{abc}	ρ_{abc}
G_1	111	$0.866\,025 \times m_1$	$1.046\,154 \times 10^2$
	122	$1.538\,842 \times m_1$	$1.463\,532 \times 10^4$
	144	$2.352\,315 \times m_1$	$1.021\,638 \times 10^7$
G_2	211	$0.587\,785 \times m_1$	$1.205\,778 \times 10^2$
	212	$0.951\,057 \times m_1$	$9.045\,125 \times 10^3$
	221	$0.951\,057 \times m_1$	$9.045\,125 \times 10^3$
	222	$1.401\,259 \times m_1$	$3.583\,739 \times 10^6$
	233	$1.817\,082 \times m_1$	$3.658\,775 \times 10^8$
G_3	311	$0.104\,528 \times m_1$	$1.130\,876 \times 10^{-1}$
	312	$0.809\,017 \times m_1$	$1.853\,066 \times 10^4$
	321	$0.809\,017 \times m_1$	$1.853\,066 \times 10^4$
	323	$1.478\,148 \times m_1$	$2.976\,315 \times 10^8$
	332	$1.478\,148 \times m_1$	$2.976\,315 \times 10^8$

field. The critical point corresponds to $t=1$, $h=0$. The masses $\tilde{m}_i$ are obtained from the eigenvalues E_i of H as $\tilde{m}_i = \xi_i^{-1} = E_i - E_0$ where E_0 is the ground-state energy. For the discrete spectrum, the masses $\tilde{m}_i$ are related to the stable particle masses m_a. We are interested in the limit $h \to 0$, $N \to \infty$ such that the scaling variable

$$\mu = hN^{15/8} \tag{7}$$

is kept fixed. We then expect a scaling form of the masses

$$\tilde{m}_i = h^{8/15} G_i(\mu). \tag{8}$$

The limit $\mu \to \infty$ then corresponds to the mass predictions in (1).

We still have to relate L with μ. To do so, we recall that conformal invariance at the critical point uniquely fixes the normalization of H [26]. For the specific form of H in (6), we must renormalize $H \to \zeta^{-1} H$ with $\zeta = 2$. Then we can write

$$m_1 L = \zeta^{-1} \tilde{m}_1(\mu \to \infty) N = \zeta^{-1} G_1(\infty) \mu^{8/15}. \tag{9}$$

The mass shifts are then calculated from (with $i = a = 1$–3)

$$\delta G_i(\mu) = (G_i(\infty) - G_i(\mu))/G_1(\infty) = -\Delta m_a(L)/m_1(\infty). \tag{10}$$

We first have to determine the $G_i(\infty)$. This involves the double extrapolation of taking first the finite-size scaling limit with μ fixed and then let $\mu \to \infty$. Computationally, it is preferable to replace this double limit by first letting $N \to \infty$ with h fixed and only afterwards extrapolate for $h \to 0$ [7, 17]. We use lattices with up to $N = 21$ sites. In table 2, we give our estimates of the $G_i(\infty)$ as a function of h along with the result of the extrapolation for $h \to 0$. The extrapolations were done with the BST extrapolation algorithm [27, 28]. From these limits, we find for the mass ratios

$$m_2/m_1 = 1.6181\ (5) \qquad m_3/m_1 = 1.994\ (5) \tag{11}$$

which improves upon earlier estimates [7, 8] and should be compared with the ratios 1.618 03 ... and 1.989 04 ... as taken from (1). Our estimates agree well with the prediction.

Table 2. Estimates for the scaling functions $G_i(\infty)$ as a function of the magnetic field h and their limits for $h \to 0$. The numbers in brackets give the estimated uncertainty in the last given digit(s). For G_1, the given numbers are exact in all given digits if $h \geq 0.30$.

h	$G_1(\infty)$	$G_2(\infty)$	$G_3(\infty)$
0.05	5.408 (4)	—	—
0.07	5.408 8 (3)	8.75 (5)	—
0.10	5.405 35 (5)	8.729 (6)	—
0.15	5.400 19 (1)	8.705 3 (4)	—
0.20	5.395 109 2 (2)	8.685 02 (4)	10.669 (3)
0.25	5.390 141 1 (2)	8.664 267 (4)	10.636 (2)
0.30	5.385 312 19	8.643 323 (2)	10.602 2 (10)
0.40	5.376 159 94	8.601 271 09 (8)	10.529 8 (8)
0.45	5.371 875 85	8.580 433 62 (4)	10.493 37 (5)
0.50	5.367 810 72	8.559 934 18 (6)	10.456 965 (30)
0.60	5.360 404 91	8.520 708 56 (2)	10.388 331 (7)
$h \to 0$	5.415 6 (3)	8.763 (4)	10.80 (5)

We now turn to the $\delta G_i(\mu)$. In comparison with the asymptotic expression $M_a^{(1)}$ of (3), μ must be large enough so that the other correction terms are still negligible. On the other hand, if μ becomes too large, the errors in our determination of $G_i(\mu)$ and $G_i(\infty)$ become larger than the value of $\delta G_i(\mu)$ itself. If μ is finite, the finite-size corrections terms can be predicted from conformal perturbation theory [8, 29]; one has

$$\tilde{m}_i = h^{8/15}(G_i(\mu) + N^{-2}R_i(\mu) + O(N^{-4})). \tag{12}$$

The regular structure of the correction terms hints at a very smooth convergence of the finite-size data. This is indeed found and the form (12) is nicely reproduced by our numerical data. In fact, the main limitation to our ability of accurately calculating $\delta G_i(\mu)$ comes from the uncertainty of the $G_i(\infty)$ because of the double limit involved in their determination. Typically, the values of $G_i(\mu)$ are known one digit more precisely than $G_1(\infty)$. To increase precision in our calculation of the $\delta G_i(\mu)$, we have therefore decided to calculate $G_2(\infty)$ and $G_3(\infty)$ by using the value of $G_1(\infty)$ from table 2 and (1), rather than taking their values from table 2.

In figure 1, we display our data for the $\delta G_i(\mu)$ as a function of $\mu^{8/15}$. First, we observe that for larger values of μ, ln $\delta G_i(\mu)$ is a linear function of $\mu^{8/15}$ as expected if only one term in (3) is contributing. This may also be considered as a test of the scaling $L \sim \mu^{8/15}$. Secondly, we compare with the full curves giving the function $M_a^{(1)}$. These functions were calculated from (3) by taking into account only those terms from table 1 where $\mu_{abc} < 2\mu_{a11}$ (see [24]). Inclusion of the other terms as well as $M_a^{(2)}$ would probably be inconsistent, since the contribution of the next order still neglected in (2) could be of the same order of magnitude. We note that the numerical values of δG_1 and δG_2 follow the predictions over two orders of magnitude. For δG_3, we have for our largest values of μ just reached the asymptotic regime described by (2).

The observed agreement with $M_a^{(1)}$ calculated as described gives, at least for this particular model, an *a posteriori* justification for neglecting $M_a^{(2)}$, which is at most of order O(exp($-m_1L$)), while at least the lowest μ_{abc} are smaller than m_1 (see table 1). We can thus conclude that our numerical data are consistent with the conjectured

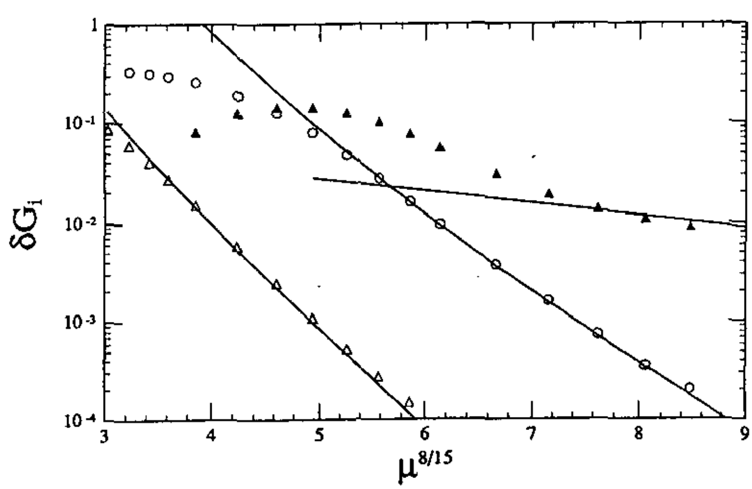

Figure 1. Comparison of the reduced mass shifts $\delta G_i(\mu)$ with the asymptotic expressions $M_a^{(1)}$ of (3) (full curves). The $M_a^{(1)}$ were calculated by taking into account only those terms from table 1 with $\mu_{abc} < 2\mu_{a11}$. G_1 corresponds to △, G_2 to ○ and G_3 to ▲.

minimal E_8 S-matrix. We have also tried to fit the numerical data to the form of (3) but with the λ_{abc} as free parameters, while the μ_{abc} were still taken from table 1. This reproduces the expected values of the λ_{a11} (with $a = 1, 2$) to within a few per cent.

Our numerical calculations are in agreement with analytical studies. From the thermodynamic Bethe ansatz [15], it is possible to calculate the central charge c of the critical, conformal invariant theory if the S-matrix of the off-critical theory is given. This method requires the integrability of the system considered. All practical calculations carried out until now have further assumed that the S-matrix is diagonal. Applying this technique to the minimal E_8 S-matrix, one finds indeed $c = \frac{1}{2}$ [6], corresponding to the Ising model. Further confirmation of the minimal S-matrix comes from comparing the thermodynamic Bethe ansatz with conformal perturbation theory for the ground state energy [15, 20], at least for systems which can be assumed to be integrable. Very recently, a truncated fermionic space approach was proposed and used to estimate mass ratios and scattering amplitudes in the 2D Ising model [30]. All these results also imply the absence of CDD-factors in the systems studied.

In summary, we have given numerical evidence that both the masses and the coupling constants estimated from the finite-size scaling functions of the two-dimensional Ising model in a magnetic field are fully consistent with the conjectured minimal S-matrix. In contrast to other techniques, the methods applied here make no assumption on the integrability of the system and can thus be applied to a far larger set of models. Further work along these lines is in progress.

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